

Positive and negative parity states of the Two-Rotor Model and scissors modes

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In previous investigations of the Two-Rotor Model with axially symmetric rotors the wave functions were assumed to be invariant under inversion of the axes of the rotors, which restricted the spectrum to positive parity states. We relax this condition requiring only that the wave functions be invariant under the square of the inversion operators. As a result we get positive as well as negative parity states that are all split by tunneling effect.

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1. *Introduction.* The Two-Rotor Model (TRM) describes the dynamics of two rigid bodies rotating with respect to each other under an attractive force around their centers of mass fixed at one and the same point. It was devised as a model for deformed atomic nuclei, in which case the rigid bodies represent the proton and neutron systems [1]. The excited states of this model were later observed in all deformed nuclei [2] and were called scissors modes.

The TRM was mostly studied for rotors with axial symmetry (the case of triaxial deformation was considered in [3]). In this case the independent variables are the unit vectors $\hat{\zeta}_1, \hat{\zeta}_2$ in the (oriented) directions of the symmetry axes of the rotors. The Two-Rotors system is invariant under inversion of each of these vectors. Previous investigations of the model were done under the restrictive assumption that also the wave functions be invariant under these inversions. As a result all the eigenstates are of positive parity. In the present paper we remove this restriction. Actually in general such inversions change the members of a degenerate multiplet into one another and the wave functions must only be eigenfunctions of their squares. We will see that under such more general condition there are also negative parity states and moreover all (positive as well as negative parity) states are split by a tunneling effect.

Very recently the TRM was adopted also as a model for single domain magnetic nanoparticles. These objects consist of a magnetic structure, called macrospin, that can rotate in a non magnetic lattice. They have been represented as a couple of rigid rotors, one associated with the nonmagnetic lattice, and the other one, with a spin attached, with the macrospin [4]. The case in which the nonmagnetic lattice is stuck in a rigid matrix is very similar to several other systems for which scissors modes have been predicted [5] (but observed until now only in Bose-Einstein condensates [6]), the similarity being especially close for ions with spin-orbit locking [7]. In all these cases one of the blades of the scissors must be identified with a cloud of moving particles and the other one with a structure at rest (the macrospin and the stuck nonmagnetic lattice respectively for nanoparticles). Nanoparticles stuck in a rigid matrix were studied in detail by such a model, and the magnetic susceptibility

was found compatible with a vast body of experimental data and in some cases the agreement was surprisingly good [4].

The cases in which the nanoparticles are free [8] or their nonmagnetic lattice is stuck in an elastic matrix have instead a close correspondence with atomic nuclei but with some important differences. Nanoparticles are not invariant with respect to inversion of the macrospin axis, and unlike atomic nuclei, the moments of inertia of nonmagnetic lattice and macrospin can be very different from each other. Application of the TRM to nanoparticles free or stuck in an elastic matrix requires therefore a little further work, but the present results should be qualitatively relevant to such systems as well.

In order to make the paper a minimum self contained we report the relevant features of the TRM.

2. *The Two Rotor Model.* The Hamiltonian in the reformulation of the model of Ref. [9] is

$$H = \frac{1}{2\mathcal{I}_1} \vec{L}_1^2 + \frac{1}{2\mathcal{I}_2} \vec{L}_2^2 + V \quad (1)$$

where \vec{L}_1, \vec{L}_2 , $\mathcal{I}_1, \mathcal{I}_2$ are the angular momenta and moments of inertia of the two rotors and V the potential interaction between them. The direction cosines of $\hat{\zeta}_1, \hat{\zeta}_2$ can be replaced by the Euler angles α, β, γ that describe the system as a whole plus the angle θ between the rotor axes

$$\cos(2\theta) = \hat{\zeta}_1 \cdot \hat{\zeta}_2. \quad (2)$$

To this end we define the frame of axes

$$\hat{\xi} = \frac{\hat{\zeta}_2 \times \hat{\zeta}_1}{2 \sin \theta}, \quad \hat{\eta} = \frac{\hat{\zeta}_2 - \hat{\zeta}_1}{2 \sin \theta}, \quad \hat{\zeta} = \frac{\hat{\zeta}_2 + \hat{\zeta}_1}{2 \cos \theta}. \quad (3)$$

The correspondence $\{\hat{\zeta}_1, \hat{\zeta}_2\} = \{\alpha, \beta, \gamma, \theta\}$ is one-to-one and regular for $0 < \theta < \frac{\pi}{2}$. The variables $\alpha, \beta, \gamma, \theta$ are not sufficient to describe the configurations of the classical system, but they describe uniquely the quantized system owing to the constraints

$$\vec{L}_1 \cdot \hat{\zeta}_1 = 0, \quad \vec{L}_2 \cdot \hat{\zeta}_2 = 0 \quad (4)$$

necessary for rigid bodies with axial symmetry. These constraints are automatically satisfied if we take the wave functions to depend on $\hat{\zeta}_1, \hat{\zeta}_2$ only.

The Two-Rotor system has an \mathcal{R} invariance consisting in the rotation through π around the ξ -axis, that is equal to the inversion of both symmetry axes and the parity operation

$$\mathcal{R} = \mathcal{I}_{\zeta_1} \mathcal{I}_{\zeta_2} = \mathcal{P}. \quad (5)$$

In many cases in the presence of an \mathcal{R} -symmetry there is a redundancy of variables because the corresponding operation can be realized acting on the intrinsic as well as on the global variables (the Euler angles). Such a redundancy must then be eliminated by an appropriate constraint. This does not happen with our variables, because the correspondence $\{\hat{\zeta}_1, \hat{\zeta}_2\} = \{\alpha, \beta, \gamma, \theta\}$ is one-to-one: indeed the intrinsic variable is θ that does not change inverting both $\hat{\zeta}_1$ and $\hat{\zeta}_2$, so that the \mathcal{R} -operation can be performed only acting on the Euler angles.

In order to express the Hamiltonian in the new variables we define the operators

$$\vec{L} = \vec{L}_1 + \vec{L}_2, \quad \vec{\mathcal{L}} = \vec{L}_1 - \vec{L}_2. \quad (6)$$

\vec{L} is the total orbital angular momentum acting on the Euler angles α, β, γ , while $\vec{\mathcal{L}}$ is not an angular momentum, and has the representation [1]

$$\vec{\mathcal{L}}_\xi = i \frac{\partial}{\partial \theta}, \quad \vec{\mathcal{L}}_\eta = -\cot \theta \vec{L}_\zeta, \quad \vec{\mathcal{L}}_\zeta = -\tan \theta \vec{L}_\eta. \quad (7)$$

The transformed Hamiltonian is the sum of the rotational Hamiltonian of the Two-Rotors system as a whole plus an intrinsic Hamiltonian

$$H = \frac{\vec{\mathcal{L}}^2}{2\mathcal{I}} + H_I \quad (8)$$

where $\mathcal{I} = \mathcal{I}_1 \mathcal{I}_2 / (\mathcal{I}_1 + \mathcal{I}_2)$ and

$$H_I = \frac{1}{2\mathcal{I}} \left[\cot^2 \theta \mathcal{L}_\zeta^2 + \tan^2 \theta \mathcal{L}_\eta^2 - \frac{\partial^2}{\partial \theta^2} - 2 \cot(2\theta) \frac{\partial}{\partial \theta} \right] + \frac{\mathcal{I}_1 - \mathcal{I}_2}{4\mathcal{I}_1 \mathcal{I}_2} \left[-\tan \theta \mathcal{L}_\zeta \mathcal{L}_\eta - \cot \theta \mathcal{L}_\eta \mathcal{L}_\zeta + i \mathcal{L}_\zeta \frac{\partial}{\partial \theta} \right] + V. \quad (9)$$

The range of θ can be separated into two regions

$$s_I = s(\theta) s\left(\frac{\pi}{4} - \theta\right), \quad s_{II} = s\left(\frac{\pi}{2} - \theta\right) s\left(\theta - \frac{\pi}{4}\right), \quad (10)$$

where $s(x)$ is the step function: $s(x) = 1, x > 0$ and zero otherwise. They are obtained from each other by the reflection of θ with respect to $\pi/2$. It is convenient to introduce the notation

$$R_\theta f(\theta) = f\left(\frac{\pi}{2} - \theta\right) = \overset{\circ}{f}(\theta), \quad (11)$$

so that $\overset{\circ}{s}_I = s_{II}$. We assume $\overset{\circ}{V} = V$, as appropriate to the geometry of the system.

The total Hamiltonian is invariant under separate inversions of the rotors axes that can be represented as

$$\mathcal{I}_{\zeta_1} = R_\zeta(\pi) R_\xi\left(\frac{\pi}{2}\right) R_\theta, \quad \mathcal{I}_{\zeta_2} = R_\eta(\pi) R_\xi\left(\frac{\pi}{2}\right) R_\theta \quad (12)$$

where $R_\zeta(\pi), R_\eta(\pi), R_\xi(\frac{\pi}{2})$ are rotation operators around the intrinsic axes.

Because in our systems the angle between the symmetry axes is very small we can assume for the potential the harmonic approximation

$$V = \frac{1}{2} C \theta_0^2 x^2 s_I + \frac{1}{2} C \theta_0^2 y^2 s_{II} \quad (13)$$

where

$$\theta_0 = (\mathcal{I}C)^{-\frac{1}{4}}, \quad x = \frac{\theta}{\theta_0}, \quad y = \frac{1}{\theta_0} \left(\frac{\pi}{2} - \theta \right). \quad (14)$$

The second term of H_I is small if $|\mathcal{I}_1 - \mathcal{I}_2| \ll 4\mathcal{I}_1 \mathcal{I}_2$ and or $\theta_0^2 \ll 1$, conditions that are both satisfied for atomic nuclei but not for nanoparticles. Nevertheless for the sake of simplicity it will be neglected in the sequel. The Hamiltonian becomes then invariant also under the transformation

$$R = R_\xi\left(\frac{\pi}{2}\right) R_\theta. \quad (15)$$

We eliminate the linear derivative in the first term of H_I by the transformation

$$(U\Phi)(\theta) = \frac{1}{\sqrt{2\sin(2\theta)}} \Phi'(\theta). \quad (16)$$

getting

$$H'_I = U H_I U^{-1} = \frac{1}{2\mathcal{I}} \left[-\frac{d^2}{d\theta^2} - (2 + \cot^2(2\theta)) + \cot^2 \theta \mathcal{I}_\zeta^2 + \tan^2 \theta \mathcal{I}_\eta^2 \right] + V(\theta). \quad (17)$$

The harmonic approximation makes more evident that the above is essentially a double well Hamiltonian. The energy splitting can be estimated by the WKB approximation

$$\delta E \approx E \int_{-\theta(E)}^{\theta(E)} \exp(-|p(\theta)|) \quad (18)$$

where $\theta(E)$ is the angle of inversion of the classical trajectory of energy E and $p(\theta)$ its conjugate momentum, $|p| = \sqrt{2\mathcal{I}(E - V)} \approx |\sin \theta|/\theta_0^2$. Because $\theta(E) \approx \theta_0$ for the states of interest

$$\delta E \approx E \exp\left(-\frac{2}{\theta_0^2}\right). \quad (19)$$

For atomic nuclei in the rare earth region $\theta_0^2 \sim 0.01$ and such energy splitting is to all effects negligible, but the situation is different for nanoparticles. The compatibility of the following results with phenomenology will be discussed at the end of the paper.

We impose the normalization

$$\int_0^{2\pi} d\alpha \int_0^\pi d\beta \sin \beta \int_0^{2\pi} d\gamma \int_0^{\frac{\pi}{2}} d\theta |\Psi_{I^\pi M K \sigma}|^2 = 1 \quad (20)$$

where I, M, K are the nucleus total angular momentum, its component on the z -axis of the laboratory system and its positive component on the ζ -axis of the intrinsic frame respectively.

In the present paper we study only the lowest states with $J = 0, 1$. The eigenfunctions and eigenvalues of H'_I in region I are then [9]

$$\begin{aligned}\varphi_K(x) &= \sqrt{\frac{1}{\theta_0}} x^{K+\frac{1}{2}} e^{-\frac{1}{2}x^2} \\ \epsilon_K &= \hbar\omega(K+1), \quad \omega = \sqrt{\frac{C}{I}}\end{aligned}\quad (21)$$

with normalization

$$\int_0^\infty dx (\varphi_K(x))^2 = \frac{1}{2}. \quad (22)$$

Positive parity states. Consider the states

$$\Psi_{I+MK\sigma} = \mathcal{F}_{MK}^I(\alpha, \beta, \gamma) \Phi_{I+K\sigma}(\theta) \quad (23)$$

where

$$\mathcal{F}_{MK}^I = \sqrt{\frac{2I+1}{16(1+\delta_{K0})\pi^2}} (\mathcal{D}_{MK}^I + (-1)^I \mathcal{D}_{M-K}^J). \quad (24)$$

Because

$$I_\zeta^2 \mathcal{F}_{M,1}^1 = I_\eta^2 \mathcal{F}_{M,1}^1 = \mathcal{F}_{M,1}^1, \quad I_\zeta^2 \mathcal{F}_{0,0}^0 = I_\eta^2 \mathcal{F}_{0,0}^0 = 0 \quad (25)$$

the Φ 's satisfy the eigenvalue equation

$$\begin{aligned}\left\{ \frac{1}{2I} \left[-\frac{\partial^2}{\partial \theta^2} + \cot^2 \theta + \tan^2 \theta - (2 + \cot(2\theta)) \right] \right. \\ \left. + V - E_{I+K\sigma} \right\} \Phi_{I+K\sigma}(\theta) = 0\end{aligned}\quad (26)$$

that is symmetric under the reflection R_θ . Neglecting the tunneling we then find

$$\begin{aligned}\Phi_{1+,1,\sigma} &= s_I \varphi_1 + \sigma s_{II} \overset{\circ}{\varphi}_1 \\ \Phi_{0+,0,\sigma} &= s_I \varphi_0 + \sigma s_{II} \overset{\circ}{\varphi}_0\end{aligned}\quad (27)$$

$$E_{1+,1,\sigma} = 2\hbar\omega, \quad E_{0+,0,\sigma} = \hbar\omega. \quad (28)$$

For each value of J, K we have a doublet whose members are distinguished by σ according to

$$R_{\zeta_1} \Psi_{I+MK\sigma} = R_{\zeta_2} \Psi_{I+MK\sigma} = R \Psi_{I+MK\sigma} = \sigma \Psi_{I+MK\sigma} \quad (29)$$

and therefore according to (5) have positive parity. Here we are confronted with the puzzling result that the ground state is degenerate, a point that will be discussed at the end.

The amplitudes of magnetic dipole transitions are

$$\begin{aligned}B(M1; 0^+, \sigma \leftrightarrow 1^+, \sigma) &= 0 \\ B(M1; 0^+, \sigma \rightarrow 1^+, -\sigma) &= B(M1) \uparrow_{scissors}. \quad (30)\end{aligned}$$

Negative parity states. The situation is different for negative parity states. Firstly it is easy to check that there is no $J^\pi = 0^-$ state. Next consider the states

$$\Psi_{1-MK\sigma} = F_{MK}^1(\alpha, \beta, \gamma) \Phi_{1-,K,\sigma}(\theta) \quad (31)$$

where

$$\begin{aligned}F_{M,1}^1 &= \sqrt{\frac{3}{16\pi^2}} (\mathcal{D}_{MK}^1 + \mathcal{D}_{M-K}^1) \\ F_{M,0}^1 &= \sqrt{\frac{3}{16\pi^2}} \mathcal{D}_{M0}^1.\end{aligned}\quad (32)$$

Because

$$\begin{aligned}I_\zeta^2 F_{M,1}^1 &= F_{M,1}^1, \quad I_\eta^2 F_{M,1}^1 = 0 \\ I_\zeta^2 F_{M,0}^1 &= 0, \quad I_\eta^2 F_{M,0}^1 = F_{M,0}^1\end{aligned}\quad (33)$$

the Φ 's satisfy the eigenvalue equations

$$\begin{aligned}\left\{ \frac{1}{2I} \left[-\frac{\partial^2}{\partial \theta^2} + \cot^2 \theta - (2 + \cot(2\theta)) \right] \right. \\ \left. + V - E_{1-,1,\sigma} \right\} \Phi_{1-,1,\sigma}(\theta) = 0\end{aligned}\quad (34)$$

$$\begin{aligned}\left\{ \frac{1}{2I} \left[-\frac{\partial^2}{\partial \theta^2} + \tan^2 \theta - (2 + \cot(2\theta)) \right] \right. \\ \left. + V - E_{1-,0,\sigma} \right\} \Phi_{1-,0,\sigma}(\theta) = 0\end{aligned}\quad (35)$$

for $K = 1, 0$ respectively. The above equations are changed into each other by the reflection R_θ . The Φ 's fall again into doublets, but since the above equations are no longer separately symmetric under R_θ , neglecting the tunneling each member of each doublet is localized in one of the wells

$$\begin{aligned}\Phi_{1-,0,+} &= s_I \sqrt{2} \varphi_0, \quad \Phi_{1-,1,+} = s_{II} \sqrt{2} \overset{\circ}{\varphi}_0 \\ \Phi_{1-,0,-} &= s_{II} \sqrt{2} \overset{\circ}{\varphi}_1, \quad \Phi_{1-,1,-} = s_I \sqrt{2} \varphi_1.\end{aligned}\quad (36)$$

Because of that, the energy splitting between the doublets is large

$$\begin{aligned}E_{1-,1,+} &= E_{1-,0,+} = \hbar\omega \\ E_{1-,1,-} &= E_{1-,0,-} = 2\hbar\omega.\end{aligned}\quad (37)$$

Here we are confronted with another puzzling result, namely that the intrinsic energy of the lower doublet is degenerate with the ground state. Also this point will be discussed below. Notice that, at variance with the positive parity states, the members of each doublet have the same σ and different K (see the Table). They are changed into one another by the inversion operators $\mathcal{I}_{\zeta_{1,2}}$

$$\begin{aligned}\mathcal{I}_{\zeta_{1,2}} \Psi_{1-M1\sigma} &= \sigma i \Psi_{1-M0\sigma} \\ \mathcal{I}_{\zeta_{1,2}} \Psi_{1-M0\sigma} &= -\sigma i \Psi_{1-M1\sigma}\end{aligned}\quad (38)$$

and by the operator R defined in (15). According to (5) all these states have therefore negative parity, but

quantum numbers	J^π	K	σ	excitation energy
ground state	0^+	0	\pm	0
scissors modes	1^+	1	\pm	$\hbar\omega + \hbar^2/\mathcal{I}$
	1^-	0,1	$+$	\hbar^2/\mathcal{I}
	1^-	0,1	$-$	$\hbar\omega + \hbar^2/\mathcal{I}$

TABLE I: Quantum numbers and excitation energies of all the states of the TRM with $J = 0, 1$.

nevertheless the electric dipole transition amplitudes to the $0^+, \sigma$ states vanish. Indeed relative rotations of rigid bodies can generate a magnetic dipole moment but not an electric one. The higher doublet, however, can decay by a magnetic dipole transition to the lower one with strength

$$B(M1; (1^-, 0, -) \rightarrow (1^-, 1, +)) = \frac{1}{2} B_{\downarrow \text{scissors}} \\ = B(M1; (1^-, 1, -) \rightarrow (1^-, 0, +)) . \quad (39)$$

Conclusion. We have determined all the states of the TRM with $J = 0, 1$. The previously known $J^\pi = 0^+, 1^+$ states are split and there are new scissors modes with $J^\pi = 1^-$ that also occur in doublets. We first discuss our findings for atomic nuclei strictly within the TRM and then their possible relevance to phenomenology. At the end some comments relative to nanoparticles.

The TRM gives for atomic nuclei the very peculiar result that with the phenomenological value of $\theta_0^2 \sim 10^{-2}$ the tunneling is altogether negligible, and the ground state splits into 2 degenerate states $J^\pi = 0^+, \sigma = \pm$. These states could be separated at a temperature $T_t \sim \delta E/k_B$, (k_B the Boltzmann constant), at which tunneling becomes important, but this temperature is altogether unreachable. Such a degeneracy, however, as far as we can see, does not give rise to any observable effect. Indeed at any reachable temperature the two $J^\pi = 0^+, \sigma = \pm$ states are equally populated, and they give rise to equal absorption cross sections whose sum equals the cross section in the absence of splitting.

The negative parity states in the framework of the TRM do not have finite transition amplitudes to the positive parity states, but can be reached in the decay of higher lying excited states (called overtones because of

the harmonic approximation). We considered [10] the possible existence of 0^+ and 2^+ overtones with intrinsic energy $2\hbar\omega$. This conjecture was rather optimistic, in view of the modest collectivity and substantial fragmentation of scissors modes, but it was supported by the fact that such states would be below threshold for neutron emission, and therefore would have a small width of purely electromagnetic nature. Such overtones, if they exist, together with their negative parity partners, should decay to the 1^- states by M1, M2 and E2 transitions.

Even if the overtones do not exist as collective modes, but the 1^- states do exist, they should be reachable by the decay of higher lying (noncollective) states. In this connection we remind that the scissors modes observed so far are affected by a substantial fragmentation, the fragments often spreading over more than 0.5 MeV around an energy of about 3 MeV. A similar fragmentation should be expected for the negative parity states, so we do not need to observe any puzzling degeneracy, and essentially the only new thing we can expect is some concentration of magnetic strength for 1^- states of energy close to that of the observed scissors modes.

It would obviously be most interesting to compare with realistic models. We expect that the situation is essentially the same in the IBA [11], whose Hamiltonian in the boson coherent state approximation exactly coincides with that of the TRM [12], so that the physical states will also be selected according to the required symmetries.

We emphasize that the degeneracy discussed above is not intrinsic to the TRM, but depends on the value of θ_0 for atomic nuclei. Indeed such degeneracy is absent for nanoparticles, whose symmetry and parameters are quite different from those of atomic nuclei. Qualitatively we can use the above results and deduce that for several nanoparticles the tunneling temperature is of the order of 1 K, a temperature that has already been reached in a number of experiments. The splitting of doublets becomes then observable. At lower temperatures only the $0^+, \sigma = +$ state should be populated, so that reaching the tunneling temperature from below we should observe a sharp increase in the magnetic susceptibility due to the contribution of the $0^+, \sigma = -$ state. These considerations will be quantitatively elaborated in a future work.

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